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COMMENTARY

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Key Points:

- Information Physics reconciles and generalizes statistical, geometric, and mechanistic views on information and Entropy
- Statistical uncertainty stems from dynamic diversity and in turn from Entropy production, with information metrics having a physical meaning
- Information metrics can be developed to enable the study of far-from-equilibrium structural-functional coevolution in hydrology and Earth system dynamics

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Debates: Does Information Theory Provide a New Paradigm for Earth Science? Emerging Concepts and Pathways of Information Physics

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Abstract Entropy and Information are key concepts not only in Information Theory but also in Physics: historically in the fields of Thermodynamics, Statistical and Analytical Mechanics, and, more recently, in the field of Information Physics. In this paper we argue that Information Physics reconciles and generalizes statistical, geometric, and mechanistic views on information. We start by demonstrating how the use and interpretation of Entropy and Information coincide in Information Theory, Statistical Thermodynamics, and Analytical Mechanics, and how this can be taken advantage of when addressing Earth Science problems in general and hydrological problems in particular. In the second part we discuss how Information Physics provides ways to quantify Information and Entropy from fundamental physical principles. This extends their use to cases where the preconditions to calculate Entropy in the classical manner as an aggregate statistical measure are not met. Indeed, these preconditions are rarely met in the Earth Sciences due either to limited observations or the far-from-equilibrium nature of evolving systems. Information Physics therefore offers new opportunities for improving the treatment of Earth Science problems.

1. Introduction

1.1. Key Take on the Debate

In the present contribution to the debate series on whether information theory provides a new paradigm for Earth Science, we argue that, on one hand, the traditional statistical and thermodynamic views on information are already well-established in the Earth and Environmental sciences, but on the other hand the information theoretic perspective has not become ubiquitous therein. Further, it has not yet provided a finished methodological product to address Earth science problems. Accordingly, we invoke essential challenges and opportunities for further improvement in how information-theoretic principles are formulated in theory and used in practice.

To overcome the limitations of classical information theory and to broaden its applicability and strength, we propose new approaches and pathways at both fundamental and applied levels. We do so by looking directly into the underlying physics, ultimately leading to a novel framework that takes the emerging discipline of *Information Physics* beyond its status quo of information-based physics (physics “made of” information), to explore a new side of it as physically based information (information “made of” physics). Along the way, we establish links to hydrology and the broader Earth system sciences.

At a more fundamental level, we argue that fundamental Physics is what underlies the statistical principles of Information Theory. In other words, the information laws are not arbitrary and reflect the core principles of Thermodynamics and Statistical Physics. This may appear to contradict the argument that information is what may lie at the foundation of physics, as noted in the cover article of this debate series (Kumar and Gupta, 2020). However, that is not quite the case. By having a fundamental physical nature underlying information at its essence, a physical reality emerging from information will still be inherently physical. In the “it from (qu-) bit” view of the world, the physical “it” is made of quantum information units “qu-bit,” which

actually correspond to quantum mechanical entities at the root of all physical phenomena. If information is not physical, then quantum mechanics and all the edifice of modern physics (across all scales from particle physics to astrophysics and cosmology) will be rendered nonphysical either, since all physics are particular cases of the more general quantum theory, which is no longer confined to microphysical phenomena. Moreover, it is also worth noting that quantum information is at the core of quantum technologies that are bringing major breakthroughs revolutionizing the technological treatment of earth science problems, such as environmental sensing, big data analytics, and high-performance computing, just to name a few. In what follows, we will focus on the physics underlying information at its essence, including how that helps to shed dynamic understanding and elicit underlying mechanisms on environmentally relevant phenomena.

1.2. From Information Theory to Information Physics

Since the inception of the Mathematical Theory of Communication by Claude Shannon in 1948 (Shannon, 1948), a vast theory has unfolded to formulate and optimize the quantification of information and its transfer across communication systems. Applications have ranged from signal processing and information flow over computer networks (Ahlsweide et al., 2000) to eliciting predictive ability across complex natural systems, including in the earth and environmental sciences (e.g., Nearing & Gupta, 2015; Neuper & Ehret, 2019; Pires & Perdigão, 2007; Ruddell & Kumar, 2009). Information Theory has become a scientific field in its own right, and has ventured into broader paradigms boosted by quantum information and computation (Nielsen & Chuang, 2002), developments in nonlinear dynamics (Nicolis & Nicolis, 2007), and the synergy between those fields (Perdigão, 2017a, 2018). Ultimately, information began to permeate across the whole edifice of scientific endeavor, leading to physics itself to be conceptualized in terms of information, resulting in the nascent field of *Information Physics*, deeply connected to statistical mechanics and thermodynamics.

In our present contribution to the debate, we take aim beneath the statistical mechanic envelope of information to unveil fundamental physics within. This brings out a new facet of Information Physics that can be understood as the *scientific quest for the fundamental physical nature of information*, and therefore entails the characterization of information from a perspective that goes beyond those of statistics and thermodynamics. In doing so, it brings out a deeper understanding about why information is the way it is and why it behaves the way it does, thereby leading to more robust methodologies for information quantification, storage, transmission and optimization, and opening new avenues laid down by the very same physics that governs information dynamics in the first place.

We argue that this perspective enables a powerful new framework to address interdisciplinary problems across the Earth sciences in general and Hydrology in particular. We see the key benefits as being

1. An ability to disentangle underlying physical mechanisms at the descriptive and inferential levels, and also at the explanatory level linking observations to fundamental dynamical principles
2. Linkage between uncertainty quantification and the underlying dynamical mechanisms of a system
3. Linkage between statistical information-theoretic perspectives on causality and the physical nature of causal mechanisms (arising from fundamental physics)
4. An ability to characterize complex hydrologic phenomena using relatively simple architectures (data or model structures) without loss of information, through dynamic source analysis rather than dimensionality reduction.

We begin by reviewing the classical links between information theory and thermodynamics, and then move on to the more novel aspects of Information Physics that will help to drive the Earth sciences forward.

2. The Dual Roots of Entropy

As described in the cover paper to this debate (Kumar & Gupta, 2020), the term entropy was coined in two fields, Thermodynamics and Information Theory, and their separate treatment has been a long-lasting source of confusion. Entropy originated in Thermodynamics as a physical quantity in the context of heat engine design by the work of Carnot, Kelvin, Joule, and Clausius. In that context Clausius showed that total thermodynamic Entropy cannot decrease, which is today known as the Second Law of Thermodynamics.

While Clausius predicted that a system evolves such that its Entropy increases, Gibbs later predicted that systems evolve in such a way that the Entropy increases as much as possible subject to the known constraints.

Gibbs realized that this solution was not based on deductive reasoning, but instead was based on inductive reasoning that the system would evolve to the most probable state.

Boltzmann added a probabilistic reinterpretation of thermodynamic entropy as an aggregate statistical descriptor of macroscale behavior in many-body problems: when calculating the volume W of an ideal gas in phase space (the space comprising the state variables and their conjugated momenta, i.e., their rates of change) he found that it had the same mathematical behavior as the Entropy. This finding led to Boltzmann's famous equation stating that the Entropy, S , of a macroscopic thermal state is a measure of the phase space volume W occupied by all microstates compatible with the macroscopic state:

$$S = k_B \log W. \quad (1)$$

The above equation enables one to interpret Gibbs' result that a system evolves to maximize the Entropy in a new way—the most probable macroscopic state of a system is the one occurring in the greatest number of ways! In other words, the Entropy of a system is directly related to the uncertainty of our knowledge about which microstate the system will be in upon observation. At the same time, it is still related to the dynamic diversity of ways in which the underlying physical system is manifested. The notions of statistical uncertainty and intrinsic physical diversity thus provide a first basic link between Entropy as an uncertainty measure and as dynamic diversity in a physical sense.

The conception of Entropy as a measure of uncertainty is argued to result in a broader foundation with wider applications (Caticha, 2012; Caticha, 2014; Dewar, 2009; Jaynes, 1982; Kleidon & Lorenz, 2005; Knuth, 2003; Lorenz et al., 2001; Phillips et al., 2006). Furthermore, it is also true that there are a growing number of scientists who consider a number of physical variables, in addition to Entropy, to be observer-based descriptions of the relationship between the system and the observer (Caticha, 2012; Goyal, 2012; Knuth, 2010; Knuth, 2014). Entropy is further argued to depend on the resolution (level of detail) in which the system is being observed or characterized, including the required resolution of model predictions (see, e.g., Tseng & Caticha, 2002).

Interpreting Entropy as a measure of uncertainty provides one traditional link between its use in physics to its use in Information Theory. Here information Entropy (in this context represented by ' H ' rather than ' S ') is used as an aggregate measure of spread of a probability distribution constructed from a collection of data, where the data are considered random and independent realizations from an underlying, stationary data-generating system. More literally, Entropy can be interpreted as the average uncertainty about the outcome of a random draw from this probability distribution (Shannon, 1948). Information i then is a measure of uncertainty reduction when receiving a particular observation from that system, which is related to the probability p of the particular occurrence (see also section 3 in the cover article Kumar & Gupta (2020)).

$$i = -\log_2 p, \quad (2)$$

$$H = E(i) = \sum_{j=1}^n -p_j \log_2 p_j. \quad (3)$$

The quantity i in equation (2) above is also sometimes referred to as the *surprise*, since it quantifies how surprised one would be to observe a state that occurs with probability p . In this context, the entropy H in equation (3) can be thought of as quantifying the expected surprise one would experience by observing the system, or the degree of uncertainty about the state of the system an observer is in *before* making the observations. This definition of Entropy is fully consistent with Boltzmann's and Gibbs' considerations, being also called Boltzmann-Gibbs-Shannon entropy in the field of statistical mechanics.

Notwithstanding the formal similarities, there is a conceptual difference between the approach of Shannon (Shannon, 1948) and those of his predecessors: the latter puts the focus more on the observer's uncertainty about the state of a system due to incomplete observation rather than on the direction of its further evolution and final state. This is associated with a fundamental difference in interpretation between observations under uncertainty in a fully deterministic world, and the hypothesis that there is inherent indetermination in the natural world per se as well—a matter of active open debate that reflects on the duality of interpretations of entropy as a human construct or a natural feature of system dynamics.

3. Uses and Limitations of Entropy

3.1. Coping With Uncertainty: The Fate of Hydrologists and Earth Scientists

Uncertainty remains a crucial aspect of hydrological analysis and prediction, as is the case across other Earth scientific fields. Because the systems of interest are typically complex and include multiple and nonlinear interdependencies, while related observations are rare and influenced by many factors, hydrological problems are typically underdetermined. This renders controlled experiments that seek to isolate and investigate single cause-and-effect relationships difficult. Consequently, probabilistic and statistical methods continue to play a crucial role, including applications of Information Theory and Bayesian probability theory with maximum Entropy approaches (e.g., Singh et al., 1986; Sonuga, 1972).

Nevertheless, the existence of uncertainties does not preclude the valuable contribution of physically informed approaches, just as stochastic frameworks do not preclude the value of deterministic ones. In this sense, hybrid stochastic-dynamic frameworks are increasingly more popular across the physical sciences (e.g., Nicolis & Nicolis, 2007). These frameworks essentially combine the deterministic treatment of dynamically resolved processes with the stochastic treatment of the unresolved processes in a single model structure.

We further argue that the information-theoretic treatment of uncertainty benefits from the coherent treatment of stochastic and deterministic approaches in a more integrated manner than the state-of-the-art juxtaposition of deterministic and stochastic terms in models. In this regard, by taking nonlinear dynamic interactions and higher-order statistics into consideration, Pires & Perdigão (2007) formulated novel high-order nonlinear information metrics of high-dimensional system complexity and uncertainty, along with a corresponding nonlinear Bayesian estimation framework, and Pires & Perdigão (2015) formulated high-order information theoretic metrics and formally linked them to underlying nonlinear dynamic interactions, that is, non-Gaussian interaction information among multivariate data and underlying nonlinear wave resonance.

3.2. Maximum Entropy: A Prudent Default

The maximum Entropy principle proposed by Jaynes (1957) was quickly introduced into hydrology (Leopold & Langbein, 1962) and has become a powerful universal tool, not only for data analysis but also for understanding and modeling nonequilibrium thermodynamic systems. Instead of starting from known or assumed physical principles to derive deterministic governing equations of hydrological variables given drivers and parameters, the statistical hydrology community typically argues for starting with maximum uncertainty as the default state of knowledge, and to then reduce that uncertainty as more and more information becomes available.

Based on Gibbs' findings, the principle of maximum Entropy states that in the absence of better knowledge, a prudent assumption is to assume the probability distribution of a system state to exhibit maximum entropy subject to the constraints of known attributes. This requirement ensures that the assigned distributions do not make unwarranted assumptions. Maximum Entropy approaches are prudent in the sense of avoiding overconfidence and the (mis)use of information that is not actually available.

Even so, this does not mean that physical principles should be ignored in favor of an unconstrained entropy maximum. As stated above, the maximum is conditioned on all known constraints, and thus to underlying fundamental principles, which are in fact a form of prior information (right or wrong, they are data). Therefore, it is neither necessary nor optimal to completely discard physical principles when formulating the maximum entropy solution, but rather to constrain the latter to the existing knowledge of the former. This further sharpens the maximum entropy estimation, helping weed out physically inconsistent solutions.

In Bayesian analysis, maximum Entropy is the most familiar theoretical framework for determination of prior distributions (Jaynes, 1957; Singh, 1998). One controversial issue preventing its more widespread application is the question of how to actually construct noninformative (or ignorance) priors to be used to initiate the Bayesian analysis, and this question has been under active debate (Ghosh, 1997; Jaynes, 1968; Seaman et al., 2012). While the uniform distribution may be thought of as an obvious candidate for systems with finite support (just as Gaussian distributions are for systems with infinite support), uniform probability density functions of continuous random variables are considered problematic since they are not invariant under

change of variable. However, Wang and Bras (2012) argued that the problem is caused by the “ambiguity in the probability distribution defined directly on continuous variables” instead of a logical loophole of the Bayesian method, and the controversy disappears once a continuous variable is interpreted as a limit of discrete variables to allow the assignment of equal probability according to the Principle of Indifference (Keynes, 2004). Since sequences of discrete variables may converge to different limits, the same uniform distribution may be represented by infinitely many probability density functions depending on the continuous limits of the discrete variables. Such an interpretation of noninformative priors removes a conceptual and technical barrier to wider applicability of the Bayesian method.

3.3. Maximum Entropy Production: A Thermodynamic Guideline for Aggregate System Dynamics

Maximum Entropy assumptions are useful when estimating system properties based on limited albeit sufficient observations under the ergodicity assumption, such as those required to characterize the initial states of hydrological models and the prior distributions in Bayesian analysis. Moreover, the concept of Entropy provides a basis to formulate the fundamental dynamics of open, dissipative systems that are far from equilibrium (Kondepudi & Prigogine, 1998). In such situations, Entropy production becomes a central descriptor of system function, which explicitly incorporates the universal tendency of systems to evolve toward thermodynamic equilibrium, as stated by the Second Law, and opens the possibility to formulation and application of thermodynamics-based optimality principles to constrain and guide system dynamics.

Because most Earth systems qualify as being open and dissipative, we can make use of thermodynamic optimality principles to describe and predict their behavior. Maximum Entropy production as an organizing principle (Martyushev & Seleznev, 2006) has been used to shed light on preferential configurations for system evolution (e.g., preferential flow paths such as river networks, atmospheric rivers, or cloud convection structures). These preferential configurations emerge as dissipative structures to erode thermodynamic gradients in far-from-equilibrium complex processes in atmospheric, hydrologic, and overall Earth system dynamics (Dewar, 2005; Kleidon & Lorenz, 2005; Kleidon & Schymanski, 2008; Ozawa et al., 2003; Paltridge, 1978; Wang et al., 2015).

Its flip-side expression is the Maximum Power Principle, which states that given sufficient degrees of freedom, far-from-equilibrium systems will evolve in a preferential manner such that they maximize work done over time (power). This principle has been used to explain the organization of drainage basins and the evolution of life on the Earth in thermodynamic optimality terms (Kleidon, 2010; Kleidon et al., 2013), which then reflect on their associated higher likelihood. Thermodynamic optimality and Likelihood estimation are thus operationally linked, the former providing a first-principle based framework to inform on the latter.

Altogether, we argue that the application of Entropy-based optimality principle helps to ensure that Earth system models are built in a thermodynamically consistent manner, which greatly facilitates model coupling across Earth science disciplines. Further, it has the potential to reduce uncertainties related to building dynamical system models by (i) weeding out configurations that produce dynamics that are in disagreement with the Second Law and (ii) preferring configurations that produce dynamics in accordance with thermodynamic optimality principles.

3.4. Capitalizing on the Dual Interpretation of Entropy

Hydrological and Earth Science questions typically involve analysis and prediction of physical systems, which allows the use of methods based in a thermodynamic interpretation of Entropy. At the same time, these questions are afflicted with considerable uncertainty due to limited data, which lends them to a probabilistic treatment employing the information interpretation of Entropy. Because these interpretations coincide on a fundamental level, taking a joint perspective can help to better cope with the challenges characteristic to most hydrological and Earth Science problems (Ehret et al., 2014). Tribus (1961) showed that thermodynamic Entropy is equivalent to information Entropy for equilibrium thermodynamic systems, and Koutsoyiannis (2014) provides several examples of this dual perspective being applied to hydrological problems. Dewar (2003, 2005) and Dewar & Maritan (2014) proposed a generalization of thermodynamic Entropy production (Kondepudi & Prigogine, 1998; Ozawa et al., 2003; Paltridge, 1978) in the context of the Bayesian probability theory and Information Theory (Jaynes, 2003), and it is now understood that the mathematical expression of Entropy production depends on the specific nonequilibrium thermodynamic processes under study.

Another interesting example of the potential offered by this joint perspective is the development of a model for evapotranspiration (Wang & Bras, 2009, 2011), where the Entropy production function (referred to as dissipation function) is envisioned as not exclusively thermodynamic Entropy production and not associated with known physical variables. Instead, it is a mathematical function formulated following the maximum Entropy principle as an inference algorithm. The formulation of this model would not be possible if Entropy (and its production) were limited to an exclusively thermodynamic interpretation. Nonetheless, Entropy production in the model and its minimization do have clear physical meaning as a quantitative measure of irreversibility of a nonequilibrium system.

3.5. The Need for a Dynamical Approach to Entropy

Despite its considerable potential to improve current practice in hydrological analysis and prediction, the underlying premises of applying the concept of Entropy are either availability of a sufficiently large dataset to derive robust probabilistic estimates, or a macroscale view of systems composed of many microscale subsystems. However, both premises are easily violated in the case of sparsely observed, nonlinear evolving systems that we seek to extrapolate. Unfortunately, many urgent Earth Science problems related to global change fall into this category (Ehret et al., 2014).

In this context, the emerging field of *Information Physics* seeks to provide methods to properly address these problems. For that purpose, we argue for a third major component (besides Information Theory and Thermodynamics) to come into play—kinematic geometry (the geometry of motion)—on the grounds of dynamical system theories.

While dynamical system theories have a long history in mathematics and physics and diverse applications to the hydrological sciences (e.g., Sangoyomi et al., 1996; Sivakumar, 2000; Rodriguez-Iturbe et al., 1989, 1991), their treatment of information has remained probabilistic akin to what is done in classical thermodynamics and statistics. In fact, the dynamical system theories treated entropy production as exponential uncertainty growth associated with stochastic perturbation of a deterministic system along unstable directions (where neighboring states grow exponentially apart), a notion linked to deterministic chaos. Therefore, while the kinematic geometry of a system was deemed deterministic, entropy (and information) remained inherently probabilistic. This led to the misconception that entropy could only exist in stochastically perturbed systems but not in deterministic systems without such perturbations, thereby violating the physical thermodynamic fact that entropy is being produced in nature irrespective of how we model it.

In that sense, classical dynamical system theories and their treatments of entropy and information were essentially the same as those in classical statistical mechanics. Therefore, the vast literature on dynamical systems, including applications to the Earth sciences, was never able to address information in ways going beyond the classical probabilistic paradigm.

But this is not the fundamental point to be made here. Our argument for bringing kinematic geometry into play is fundamentally different in that our resulting information metrics do not depend on any probabilistic considerations in stochastic-dynamical systems, but rather on the fundamental nature of the physics underlying the kinematic geometry per se, for example, on the system motion and entropy production of even a single unperturbed deterministic process.

So while classical dynamical system approaches are perturbative (evaluating entropy production from how a system responds to perturbations), the kinematic geometry view is inherently physical and nonperturbative. In fact, it allows for the assessment of entropy production without having to generate an ensemble of perturbations, and without the need to disturb the system and study the propagation of its perturbations. Rather than triggering actions to measure reactions, we can learn about dynamical systems by observing and documenting entropy production as it naturally unfolds in the system, something that remained an elusive goal until the theory of dynamical systems was recently invoked.

As an early effort to motivate a tripartite unification of Information Theory, Thermodynamics, and Dynamical systems, Perdigão (2010) and Perdigão et al. (2016) developed methodological bridges across the aforementioned fields, thereby providing a physically consistent unified mathematical framework for describing and modeling system coevolution. In doing so, coevolution was clarified as “far-from-equilibrium nonergodic thermodynamic mixing” where coupling exists not only between state variables but also between state variables and dynamical laws (Perdigão, 2017a).

This attention to nonergodic dynamics brings a crucial advance relative to the classical dynamical system and thermodynamic approaches, both of which are grounded on invariants of motion such as classical physical laws and thermodynamic principles. While dynamical system theories (including “chaos theory”) and information theories (including “entropy theory”) are all founded on rigid analytical and statistical mechanics, this novel take on information physics brings into play nonergodic features such as spatiotemporal symmetry breaks and associated coevolutionary interplay.

In this regard, Perdigão & Blöschl (2014, 2015) formulated a new coevolution index from spatiotemporal asymmetry and applied it for hydrological systems, based on high-order nonlinear information-theoretical metrics proposed by Pires & Perdigão (2007) and underlying dynamical principles developed in Perdigão (2010), facilitating the thermodynamically consistent study of landscape-climate coevolution. For example, in unstable coevolutionary hillslopes, the rate of Entropy production was shown to be maximum in line with the coevolution index, while in noncoevolutionary stable basins the system remains in thermodynamic equilibrium, as seen in both data-based and physically based model design. While such approaches are still in their infancy, these initial steps encourage a journey from statistics toward the underlying physics, via the *kinematic-geometric treatment of information*, a pathway we term “Information Geometry.”

4. Information Geometry in Analytical Mechanics: From Descriptive Statistics to Underlying Physics

The advantage of linking analytical mechanics (more broadly theoretical physics) with Thermodynamics and Information Theory is that the latter can now be grounded in both kinematic geometry and probabilistic definitions. Kinematic geometry represents the time variation of system variables in the mathematical “phase space” that describes the state variables and their conjugated momenta. This should not be confused with the “state space” that is spun by the state variables alone, and as such contains no dynamic information. An illustrative example of time series and associated phase spaces for a damped oscillator are depicted in Figure 1:

Examples of such systems can be widely found in nature. For instance, the harmonic oscillator is a minimalist idealized representation of the annual cycle in temperature, or more trivially the motion of a ceaseless pendulum. In a hydrologic context, the damped oscillator can represent the oscillation unleashed by opening a gate separating two reservoirs with different water levels, from an initial amplitude corresponding to their height difference, toward a final intermediate level corresponding to the thermodynamic equilibrium of the combined system.

The example in Figure 1 helps to illustrate how Entropy can be defined from geometric and topologic properties of the system representation in phase space rather than on purely probabilistic considerations. Topology expresses aggregate form, and kinematic geometry expresses detailed function. From a fundamental analytical mechanics perspective, Entropy can be expressed as the *energy density of the system dynamics in phase space*, that is, the energy ratio between the actual dynamic footprint of the system and the entire domain spun by all the system variables and conjugated momenta, as defined in Perdigão (2017a). As such, Entropy is intrinsically physical, while remaining fully consistent with the traditional notion that it represents the probability of the system manifesting in each unit volume of phase space. In fact, the density of the dynamics on a certain phase space region is linked to the probability that the system dynamics manifest in that region. This is further consistent with Thermodynamics, in that the more densely populated regions of system dynamics in phase space correspond to the preferential flow paths (predominant orbits in phase space) through which the system produces entropy, and so the functional evolution of such density is consistent with the second and fourth laws of thermodynamics (for the formal proof, see Perdigão (2017a)).

An intuitive notion of Entropy from kinematic geometry of the above damped oscillator example can be seen in Figure 2. The left panel depicts the phase space portrait of a damped oscillator (line spiraling inward toward the center) colored by the associated Entropy normalized relative to the maximum Entropy at thermodynamic equilibrium. The right panel depicts the corresponding normalized Entropy and Entropy production rates of the system over time. The functional time dependence of Entropy and Entropy production rates are thermodynamically consistent with Entropy growing in a convex way consistent with the Second Law, and Entropy production rate decreasing accordingly.

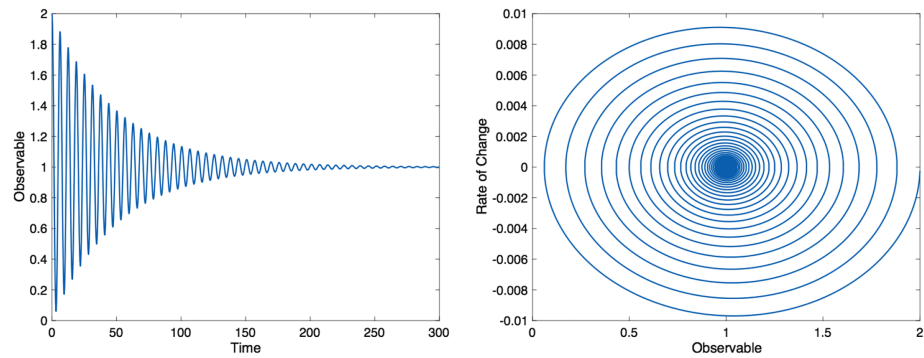


Figure 1. (left panel) Time series of a damped oscillator (e.g., a friction-afflicted pendulum). (right panel) Phase space of a damped oscillator. Figure redrawn from Perdigão (2017a).

In a hydraulic context, the aforementioned damped oscillator can be thought of as representing a system of two linked hydraulic chambers (reservoirs), where at initial time $t = 0$ the reservoirs have sharply different water levels, higher in reservoir A, and lower in reservoir B. At time $t > 0$, a wide channel connecting the bottom of the two reservoirs opens, thereby triggering water flow between the reservoirs. Given the water level contrast between the reservoirs and the large flux enabled by the wide channel, the rapid flow of water leads to the water level of reservoir B overshooting what would be an equilibrium with the water level of reservoir A. This then triggers a corrective back-flux to reservoir A, which also experiences overshoot, albeit lower than the first flux. This embodies a pendular, oscillatory water motion between the reservoirs, dampening as the overshoot fades with each oscillatory cycle, until equilibrium is reached wherein the water levels of reservoirs A and B are uniform.

This simple example illustrates how a thermodynamic potential (here the gradient in water levels) triggers entropy production until it stops when a uniform potential energy is reached (here represented by water levels). The integral of the entropy production rate through this time period corresponds to the maximum entropy possible resulting from the dissipation of the initial gradient. More importantly, it illustrates the relevance of introducing a kinematic-geometric take on Entropy and information. In spite of the exactness of the deterministic process in question there is still entropy production, and with it the production of information regarding dynamic structure. The phase space portrait is, in its essence, *dynamic information*. In this sense, from a physics perspective, information can be perceived as a realistic feature of the natural world.

So how does one reconcile the uncertainty-based statistical Entropy with the reality-based kinematic-geometric Entropy? Here one might expect the statistical Entropy to be zero given the deterministic nature of the system. This conundrum disappears once we become clear about how each perspective is actually contextualized. When we formulate statistical Entropy, we do not look at the geometry of the dynamics in phase space, but instead at the aggregate of states that characterize the entire system history—this plots as a dense

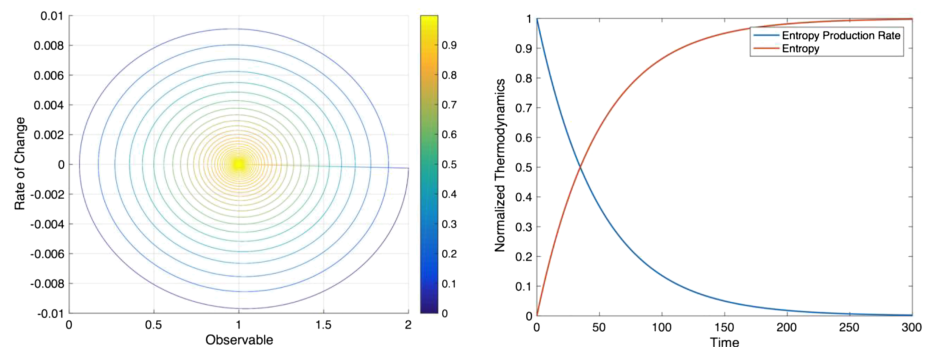


Figure 2. Phase space portrait a damped oscillator (compare to Figure 1) and associated time variation of Entropy and Entropy production rates. The color scale of the left panel is indexed to the time-varying Entropy of the system. Figure redrawn from Perdigão (2017a).

distribution of dots, each of which represents a particular stage in the system dynamics. Accordingly, the statistical Entropy of that distribution is mathematically equivalent to the integral of the kinematic-geometric entropy (phase spatial density) over the full thermodynamic time (until equilibrium). It is important to note that this correspondence holds if and only if the record of system history goes all the way until equilibrium so that the state dispersion of the system history corresponds to the kinematic-geometric track (the orbit) of the deterministic representation of the system. When that correspondence exists, the system is called *ergodic*.

Overall, therefore, there is no fundamental dichotomy between statistics and geometry: they express the same concepts, albeit in formally different ways. The purpose of a physical characterization in terms of energy is to provide a dynamic interpretation of information metrics, which neither commits to a deterministic nor to a stochastic view of the world. Meanwhile, the phase space integration of the kinematic-geometric view leads to a topological view consistent with that of ergodic dynamical system theories, in which the system is considered to be structurally invariant so that a long time series represents the phase spatial diversity.

The corresponding aggregate information metrics are analytically obtained in Perdigão (2017b) by integrating the local event-scale dynamic codependences (Perdigão et al., 2016). The resulting aggregate metrics bring out nonlinear multivariate links consistent with the multilateral non-Gaussian information-theoretical metrics of Pires & Perdigão (2015), including triadic and high-order generalizations of information-theoretic synergy and redundancy for nonlinearly interacting multivariate systems, thereby enabling kinematic-geometric aspects of complexity to be characterized either geometrically or statistically, in dynamic models or data sets.

Ultimately, whether to use the statistical or kinematic-geometry approaches is a matter of context-motivated language. If the purpose is to characterize the likelihood of microstate occurrences within a macrophysical aggregate without taking microphysical or event-scale dynamics into explicit consideration, a probabilistic approach to information makes sense. However, if the purpose is to understand the underlying dynamics at play shaping the statistics, then kinematic geometric approaches to information are particularly useful. All in all, the statistical metrics then come as being equivalent to topological envelopes of the fine-scale kinematic geometry.

5. Information Physics in Far-From-Equilibrium Structural-Functional Coevolution

As explained earlier, traditional Information Theory, Thermodynamics, and System theories are framed in terms of aggregate information obtained from statistical metrics under assumptions of ergodicity. In doing so, they aptly capture the statistical-geometric macrophysical aspects of system dynamics, while microphysical evolution of the system is constrained by structural invariants that also shape rigid thermodynamic optimality principles. In this regard, even chaos is a fundamental consequence of structural regularity in the system dynamics. So while small perturbations of a chaotic system can lead to wildly different pathways to equilibrium, the statistical physics of the end state shapes a perfectly stationary distribution consistent with thermodynamic limits and kinematic geometry in classical mechanics. Because Thermodynamic optimality principles are set in this regime of structural invariance, they can only characterize limiting conditions, maxima or minima in potential functions and their gradients, ultimately all linked to the overarching concept of free energy.

However, many complex systems (e.g., hydro-climate dynamics in the presence of climate change) of interest are typically undergoing far-from-equilibrium structural-functional coevolution. In such cases, the thermodynamic limits are not invariant but rather changing at rates faster than what quasi-static thermodynamic optimality allows, which often renders optimality principles and associated information theoretical metrics to be inadequate. Moreover, such far-from-equilibrium dynamics come with microphysical mixing that leads to event codependence. This violates the assumptions of local equilibrium and microphysical event independence. In a nutshell, the traditional Entropy functionals in Thermodynamics (Boltzmann-Gibbs Entropy) and Information Theory (Shannon Entropy) no longer hold.

To overcome these limitations, it has become necessary to generalize dynamical system theory and information theory to represent nonergodic system evolution (which has been done in detail in Perdigão et al. (2016),

Perdigão (2017a), and Perdigão (2018)). These generalizations enable a prognostic study of the collective emergence of system features beyond the predictability limits of classical dynamical systems theory, including nonrecurrent synergistic innovation, which is not possible via the classical stochastic-dynamic approach. Moreover, they facilitate the retrieval of extra information about the event-scale interdependencies from data, including far-from-equilibrium interplay elusive to traditional information metrics.

For instance, the Shannon entropy-based information theoretic metrics of a hydrologic streamflow series take the individual measurements as dynamically independent from each other, that is, as if the time series would represent a random process or a perfect gas in thermodynamic equilibrium, which is clearly not the case. In streamflows there is inherent dynamic codependence between individual states: after all, this is the core essence of a *flow*. Shannon entropy therefore takes part of the story, an aggregate statistical behavior under event-scale equilibrium, but misses the dynamic codependence and coevolution among states. Those dynamic links are then provided in the novel information physics metrics in nonlinear statistical mechanics by Perdigão (2018), including generalizations of multivariate entropy, synergy, and redundancy. These generalizations capture not only the aggregate system statistics but also how such statistics change and how the dynamic sequence unfolds within, thereby *connecting the dots* both in ergodic system dynamics and in nonergodic system coevolution.

The aforementioned information physics metrics further bring added benefits to information-theoretical causal inference by unveiling causal links among statistically independent variables, thereby capturing nonlinear noneroding causal links elusive to classical measures such as Transfer Entropy (Schreiber, 2000) that were grounded on Shannon Entropy. The derivation of the new generalized causal information metric and its applications to ocean-atmospheric and hydro-climatic causal inference are presented in detail in Perdigão (2017a).

6. Concluding Remarks and Outlook

The traditional statistical view treats Entropy as a system level (macroscopic) descriptor of the amount of information needed to characterize it. While Thermodynamics provides a physical context for the production of Entropy, in Information Theory the focus is on system encoding. So Entropy can be viewed as an uncertainty measure or a physical quantity depending on context; the physical perspective is tied to the natural metric complexity of the system (the diversity of microstates), while the statistical perspective reflects the difficulty in eliciting microstates from macrophysical descriptors. Physical Entropy then becomes a natural quantity, whereas statistical Entropy is dependent on how the system is being observed.

Beneath these concepts of Entropy lie fundamental physics, which characterizes the system behavior in terms of its underlying dynamical mechanisms. These mechanisms can be represented in the phase space of state variables and their associated conjugate momenta (rates of change). This enables Thermodynamic and Information-Theoretic considerations to be tied to the geometric properties of the system footprint in phase space. The key added value of the kinematic-geometric perspective is to capture not only the diversity of microstates and the overall topology of the system but also the dynamic sequence and mechanistic context in terms of state variables and momenta, thereby helping to elicit the underlying mechanisms at play that shape the dynamics, that is, the dynamic footprint associated with the underlying dynamic physical laws.

Still, traditional dynamical system approaches are grounded on the very same structural system invariance assumptions as Information Theory and Thermodynamics. Dynamic couplings in traditional information and dynamical system approaches are wrongly perceived as coevolution, when in reality they entail kinematic-geometric covariation of systems in ergodic balance; that is, in those paradigms the variable values change in time but the system overall does not.

For instance, coupled models such as those in classical climate dynamics and socio-hydrology prescribe time variation of local codependencies (cross-derivatives), but do not allow for the system as a whole to evolve, since the laws are rigid, grounded on ergodic invariants and any variability then comes out of artificial stochastic noise, itself devoid of evolutionary meaning. In that regard, such models enable deterministic bifurcations and intermittence between regimes, but do not allow for any true system innovation, thereby modeling long-term dynamics with laws that are only valid in the short term.

In physics, dynamic laws do not need to be deterministic in the classical Newtonian sense. While traditional dynamical system approaches in classical mechanics assume the rigidity of “invariants of motion” through stringent deterministic models, which then require stochastic ad hoc patches to reflect dynamic diversity, in the emerging nonergodic coevolutionary approaches such invariance is no longer required. In doing so, we can actually begin capturing the mechanisms underlying elusive coevolutionary features seen across Earth system dynamics.

These advances mean that rather than rigid deterministic orbits with artificially added stochastic elements for diversity, the dynamic nature of the system laws can natively produce evolutionary diversity and complexity, learning, adapting, and seeking new thermodynamic optimality targets as the evolutionary dynamics unfold (Perdigão, 2017a). In that regard, physical evolution can be seen neither as fatalist determinism nor random wandering, but rather as a learning process akin to a natural adaptive machine-learning engine, an evolutionary dynamical system being akin to a living species producing diversity on its own.

In practical applications with limited data availability, an operational challenge resides in dealing with sparse data records from which to derive kinematic-geometric and information-theoretic diagnostics. In that regard, there is a growing literature on using information theory to infer dynamical relationships among system variables (Gençaga et al., 2015; Knuth et al., 2008), and on information estimators for sparse data (Pires & Perdigão, 2013; Testa et al., 2016), including in hydrologic contexts (Liu et al., 2016; Salas et al., 2017). These efforts represent the beginning of a journey, and further methodological and applied developments are yet to come.

Ultimately, the task of mining the information physics within a system involves both the understanding of fundamental physical principles and case-specific information retrieval. Here the fundamental challenge is to “ask the right questions” about the system. While classical correlation may capture the tip of the iceberg, and information-theoretic measures may capture more features, the study of kinematic-geometric couplings will enable the study of dependency structure. The quest does not end here—for all observational and analytic paradigms the fundamental question remains one of how best to read Nature.

As also touched on by the cover paper to this debate series (Kumar & Gupta, 2020) information physics ultimately tackles the question of whether information per se is a physical quantity, or represents knowledge about a physical quantity. While one prevailing view is that knowledge about a property is not necessarily the property itself, Information Physics treats information as having a physical existence independent of knowledge. Whether or not that is indeed the case is up for debate. Nonetheless, for practical purposes, the physical conceptualization behind Information Physics enables the characterization of dynamic interdependencies at the event scale and helps to explain the physics (and in particular the kinematic geometry) that shapes the statistical history of the system. In a hydrological system under global change, this can provide a powerful approach to driving the science forward.

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Data Statement

This study does not use any observational data sets. The figures are mathematically, synthetically generated, citing the underlying references in the corresponding captions and associated text.

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